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Improving the Model Fidelity for the Mechanical Response in a Thermal Cookof of HMX

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IMPROVING THE MODEL FIDELITY FOR THE MECHANICAL RESPONSE IN A THERMAL COOKOFF OF HMX

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Abstract. Understanding the response of energetic materials to adverse thermal environments is necessary to have confidence in the safety those systems. In the past few years we have been improving our thermal-mechanical-chemical modeling of HMX/Viton-A based systems. Time to event predictions are very good, to within a degree of the experimental result. However, the chemical network/reaction rates are under constrained, and many networks can achieve the same level of accuracy. Recently, we have significantly improved the mechanical response modeling by the inclusion of porosity and surface tension in the solid species in the reaction network. Here we consider the effect of HMX sublimation on the reaction network, and also consider the effect of the trapped gas in the ullage space on the overall mechanical response of the models of experiments like the Scaled Thermal Explosion eXperiemt.

Keywords: Thermal Cookoff, HMX, LX-10, ALE3D.
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INTRODUCTION

Understanding the response of a high explosive system to a variety of off normal physical environments is fundamental to predicting the safety of such systems in various accident scenarios. One such environment is slow cookoff, where the high explosive is heated slowly over a period of several hours or days. For a thermal cookoff event, there are two aspects that need to be predicted to have confidence in one's ability to model the process: 1) time to event, and 2) strain history. To model the first aspect, all that is needed is a thermal transport code with chemical reactions to provide a heat source. There are many models that do a reasonable job of modeling the time to event. To model the second (strain history), one needs that coupled with implicit mechanics, in our case the code ALE3D, which is a coupled implicit/explicit mechanics, implicit/explicit thermal, chemical reaction code.[1]

Tarver and Tran [2] developed a model for the decomposition of HMX that was subsequently modified by Yoh et. al.[3] to model an LX-04 Scaled Thermal Explosion Experiment (STEX) [4]. In previous work, Nichols et. al. [5] further modified the reaction model and equation of state of the gaseous components, and added a porosity model to significantly improve both the time to event and the strain behavior compared to Yoh et. al. In further work, Nichols [6] examined the effect of surface tension between the HMX and the pore gas on the mechanical response.

In all of these models, the time to event prediction is uniformly good, while the strain response is uniformly high. In this paper, we consider how the presence of HMX vapor could change the response, and also consider the effect of the ullage gas.

MODELING HMX/VITON-A FOR STEX

In order to model the slow heat response of HMX/Viton-A systems (LX-04, LX-07, LX-10 with 85%, 90%, and 95% HMX respectively), we use the reaction network and rates developed in Nichols et.al. [5]. These rates are all driven by mass concentration instead of the more standard molar concentration. This is congruous with the fact that we do not know the exact molecular species involved with the reaction. The material models for the solid species β-HMX, δ-HMX, f (a solid decomposition product), and all of the thermal conductivities were developed by Yoh et.al. [3]. The gaseous species hg (the first gaseous product) and lg (final equilibrium gas product) are those developed in Nichols et.al. [5] based on the Cheetah equation of state code [7]. The hg product was assumed to be the early decomposition products like N_2O, and CH_2O. While the equations of state and reaction models are the same across the HMX/Viton-A family of explosives, we adjust the mechanical response for the initial β-HMX to match that of the particular composition. The composite material was modeled to have a 2% initial porosity. This is required to describe the initial expansion and behavior of the STEX system when the HE comes into contact with the walls. LX-10 is used in the TE-47 STEX experiment examined here.

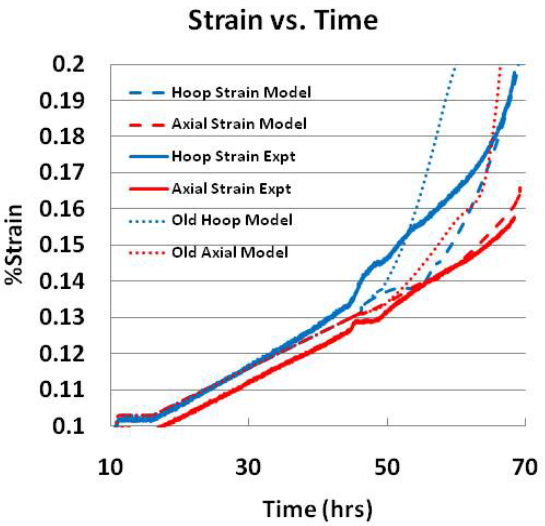

Figure 1. Comparison of the hoop and axial strain for the TE-47 STEX experiment with the initial model as described in Nichols et. al. [5] (old) and the new model where the first gas species was replaced with HMX vapor. The hoop strains are always greater than the axial strains for the same system.

Examination of Vapor Pressure of HMX

During the examination of the effect of the pore surface tension on the STEX mechanical response, we noted that the effect of the surface tension was to delay the effect of the pressurization due to the creation of HMX product gas. Since the first gas producing reaction is calibrated to TGA experiments which measure the rate of mass loss, we thought to examine the inclusion of the HMX sublimation/condensation reactions. Such reactions would provide an alternate gas production/mass loss mechanism for the unconfined experiments that would then not contribute to the pressurization of the STEX apparatus.

Several researchers have examined the vapor pressure of HMX [8,9,10]. One can fit an Arrhenius form to the vapor pressure as a function of temperature. This Arrhenius form has an activation energy of 44.1 kcal/mol. The activation energy for the first solid to gas reaction in our reaction framework is 44.3 kcal/mol. Given that both reactions are expressing the transition in the reaction network from a solid to a gas, we hypothesize that the two processes are actually one.

We modeled the change in the first gas species by increasing the reference density of the gas by a factor of 8. This corresponds to a change from 8 gaseous fragments (4 N_2O, 4 CH_2O) to a single HMX molecule. The strain response of the TE-47 STEX experiment along with the results from [5] and the new calculation are shown in Fig. 1. Note that previously the hoop strain was 0.5% at the time of the thermal excursion. With both the experiment and the new model, the hoop strain is approximately 0.2%. It is also important to note the structure between 47 and 52 hrs, where the hoop and axial strain diverge and then converge. This is due to the contact of the LX-10 with the STEX walls while it is undergoing a phase change which preferentially induces radial expansion over axial expansion.

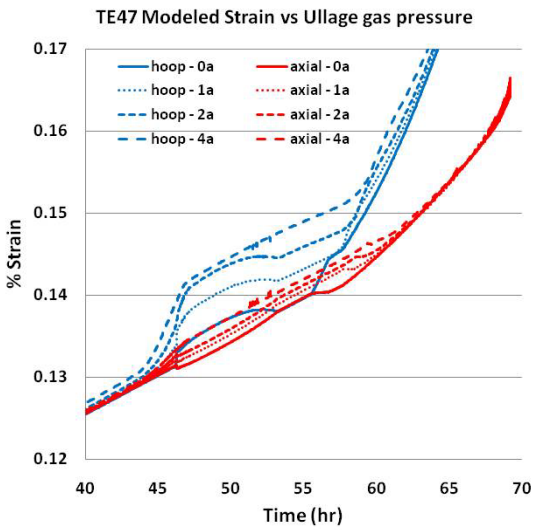

Figure 2. The effect of adding ullage gas to the simulation at 0, 1, 2, and 4 atmospheres initial pressure. Note that as the initial pressure increases, the hoop and axial strain separate before the time of HE contact (approx. 47 hrs), and that at the higher initial pressure we are starting to wash out detail in the contact region.

Modeling Ullage Gas

By comparing the stress response of the STEX experiment and the model, one can note that the model is not capturing the stress response of the STEX apparatus at early time, before the HE has made contact with the walls. From simple mechanics, it is known that the axial and hoop strain in a thin walled cylindrical vessel should be identical if the vessel is expanding due to thermal expansion, and that the hoop strain should be twice that of the axial if it is being expanded due to a internal pressure. The model is predicting identical behavior, whereas the experiment is exhibiting a small amount of pressurization response. This pressurization is undoubtedly due to a relatively small amount of gas trapped in the STEX between the HE and the walls. This strain behavior cannot be captured with the original Lagrange treatment.

There are several methods one could use to try to represent the ullage gas. One could mesh up the ullage region and fill it with gas. The problem with this approach is that the volume of the ullage gas eventually goes to zero, which would cause significant problems with a Lagrangian solution, as the courant time step condition would go to zero. Another approach would be to treat the entire region inside the walls as Eulerian, allowing the HE and the air to mix as the HE expands. This would reduce the accuracy of the solution, as mixed elements are always treated first order.

The approach taken was to define both an HE region in the vessel as well as a void region. . The void and HE regions do not interact with each other. The purpose of the void region is to compute the total volume inside the vessel, without changing the physical response. The volume of the ullage gas is computed from the difference between the void volume and the HE volume. This is then fed into an ideal gas equation of state with the time dependent temperature set to the boundary temperature. The resultant pressure is then applied as a boundary condition to the inside of the vessel and the outside of the HE.

We applied the ullage gas model to the previously defined STEX model, with an initial gas pressure of 0, 1, 2, and 4 atmospheres. The results are shown in figure 2. Note that as the initial ullage gas pressure is increased, the hoop and axial strains separate from each other. It should be noted that at an initial value of 4 atmospheres all of the detail after the HE has made contact with the walls is washed out. Since the actual system has these structures, it is clear that the gas pressurization must be less than 4 atmospheres

Final Refinements

Sufficient improvement have been made in the HMX model that approximations that had been done during its initial development are now a significant fraction of the remaining difference between it and experiment. We reconsidered the TE-47 experimental setup and adjusted the part dimensions, species densities to be in better agreement with LX-10, set the porosity to 1.9% to agree with the overall average density. One consequence of this is that the reference density of the δ-HMX and final solid species are now 6% and 7% lower, respectively, than that of the β-HMX. The results of this calculation are shown in Fig 3.

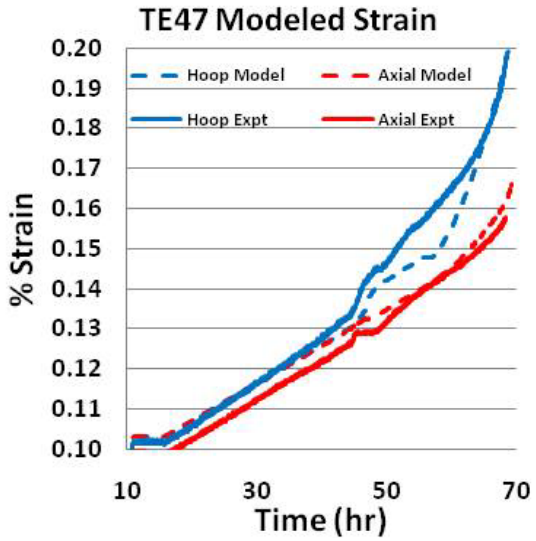

Figure 3. Final hoop and axial strain model compared to experimental results for the STEX TE-47. This model includes 1 atmosphere initial pressure ullage gas, and a slightly modified intermediate solid density. Note the significant improvement in mechanical response

CONCLUSION

We have shown that by replacing the first gaseous species in our HMX reaction network with HMX vapor, we have significantly improved the mechanical fidelity of our model for HMX/Vitan-A systems. We have also demonstrated a method for modeling the ullage gas that one generally finds in actual systems. These improvements in the modeling framework have significantly reduced the overall modeling error for the initial thermal mechanical response is comparable to the variations between experimental setups. Further tweaking of model

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